Glutaric acid, but-3-yl-2-yn 4-bromophenyl ester

Inchi: InChI=1S/C15H15BrO4/c1-3-11(2)19-14(17)5-4-6-15(18)20-13-9-7-12(16)8-10-13/h1,7-1

InchiKey: ZNUQBOCKIUAPJT-UHFFFAOYSA-N

Formula: C15H15BrO4

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 339.18

Physical Properties

Property code	Value	Unit	Source
gf	-54.69	kJ/mol	Joback Method
hf	-304.52	kJ/mol	Joback Method
hfus	38.57	kJ/mol	Joback Method
hvap	76.14	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.090		Crippen Method
mcvol	222.230	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook
tb	782.68	K	Joback Method
tc	1010.89	K	Joback Method
tf	533.84	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.47	J/mol×K	782.68	Joback Method
cpg	592.88	J/mol×K	820.72	Joback Method
cpg	604.30	J/mol×K	858.75	Joback Method
cpg	614.76	J/mol×K	896.79	Joback Method
cpg	624.30	J/mol×K	934.82	Joback Method
cpg	632.95	J/mol×K	972.86	Joback Method
cpg	640.74	J/mol×K	1010.89	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393285&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume